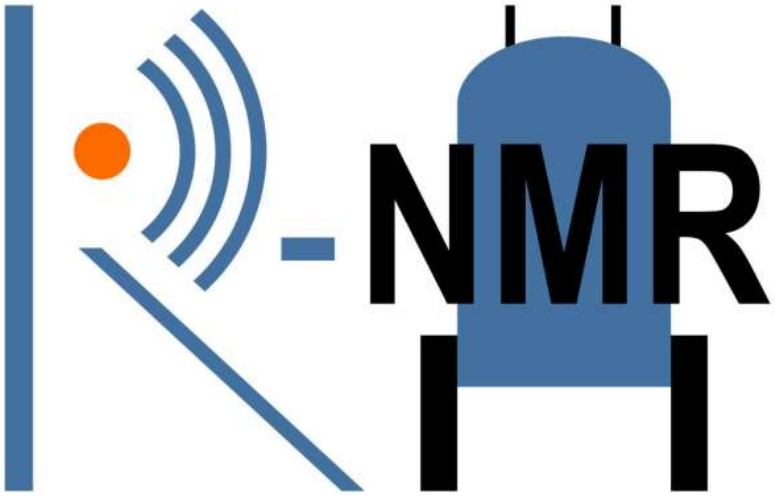

Deliverable 3.2

Procedures for the assignment of users` levels and definition of the corresponding roles of infrastructure staff

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CONTENTS

1. Introduction

This report aims to discuss and present a flexible, general solution towards the assessment of user experience levels concerning the remote control of NMR hardware based on the analysis of the responses to the NMR User Survey conducted in early 2023 (Milestone 2.2). A simple to implement, 3-tier scheme of access levels is proposed, describing increasingly advanced remote capabilities alongside corresponding responsibilities of the local operators in support of the remote users. The report will therefore be of use for the implementation of standardized experiments for remote access to liquid and solid-state NMR within WP4.

As demand for NMR measurement time increases, accommodating users with diverse expertise levels will be pivotal for the safe and efficient use of NMR hardware. Remote spectrometer access introduces distinct challenges and will require particular attention to dedicated training methods, practical assistance, hardware control, and data management.

2. Allocation of user access levels

The survey conducted in WP2 among facility managers and users has highlighted a large variety of instrumentation available, user profiles, historical practices and safety protocols. It appears therefore difficult to establish a universal method for quantifying the capacity of a given user and establish their access level. Such a decision is left in the hands of the facility managers and/or the local operators, who will have the possibility to make an informed decision based on the exchanges carried out with the users prior to the campaign of data acquisition, i.e. all along the steps of sample admission and pre-acquisition setting. Nonetheless, a standard questionnaire has been established, to guide the facility managers and/or the local operators in inquiring on the level of basic and practical NMR knowledge of the users (prior formal training, familiarity with a given spectrometer brand, types of samples worked with, hands-on experience, pulse program writing, calibration tasks, …). An example of such a questionnaire, by no means exhaustive, is provided in Appendix at the end of the current

document. It may be adapted by the facility managers and incorporated into the submission portals of any local, national or European NMR infrastructure.

3. Access level descriptions

Level 1: Monitoring only mode.

With Level 1 remote access, local operators will perform all aspects of the planned experimentation. This mode will cater for users with limited NMR expertise whose main objective is to simply collect data on their sample from the host institute. Upon prior user request, remote observation of the spectrometer control screen (strictly without control capability) should be provided by the local staff. This option could be used, for example, to provide assistance in experimental setup or for users to follow the procedures for educational purposes. Either way, users should communicate their intentions clearly in the initial experimental plans so that suitable communication channels (telephone, email, direct-message platforms etc.,) can be set up and/or connection details be shared by the local operator ahead of time.

For level 1 access, both users and local operators should ensure there is a clear understanding of the experimental expectations. In the absence of any direct communication, operators should be free to take educated reactions to common practical difficulties (i.e., low signal:noise) without input or reproach.

Level 2: Staff supervision mode.

In practice, Level 2 access will require that users are provided with procedures and credentials to initiate remote desktop connections to spectrometer computers. However, in the most general case, users should only be afforded remote access control in the presence of (or in the knowledge of a present) the local operator (see R-NMR Deliverable 3.3 for technical details). The remote user will only be able to control a limited set of experimental parameters, for example by running IconNMR module in the case of Bruker spectrometers.

Level 3: Limited-support mode.

Level 3 access will be limited to expert users only. Only the tasks that cannot be performed remotely, such as sample handling or probe exchange, will be performed by local operators. Full remote-desktop control will be provided. Whilst preconditions can of course be agreed upon beforehand, because user access can be unsupervised, all work performed should be assumed to be at the level of a trusted expert user. That is, the user would have full, unsupervised, control over the spectrometer at any time during their session without any limitation as to the commands that can be executed. This could include editing pulse programs, changing console routings, or adjusting standard pulse lengths and powers. However, hardware configuration changes and hardware rebooting will be allowed only with a prior explicit consent of the local operator. Level 3 access should therefore be treated as a serious privilege, only afforded to the most trusted and experienced users.

Nonetheless, the specific responsibilities of each party should be communicated clearly in advance. For example, despite experience, local operators could be required to perform actions mid-session due to hardware limitations (i.e., no available ATMA probes or sample changers), or for help in re-evaluating aspects such as tube positioning or magic-angle calibration.

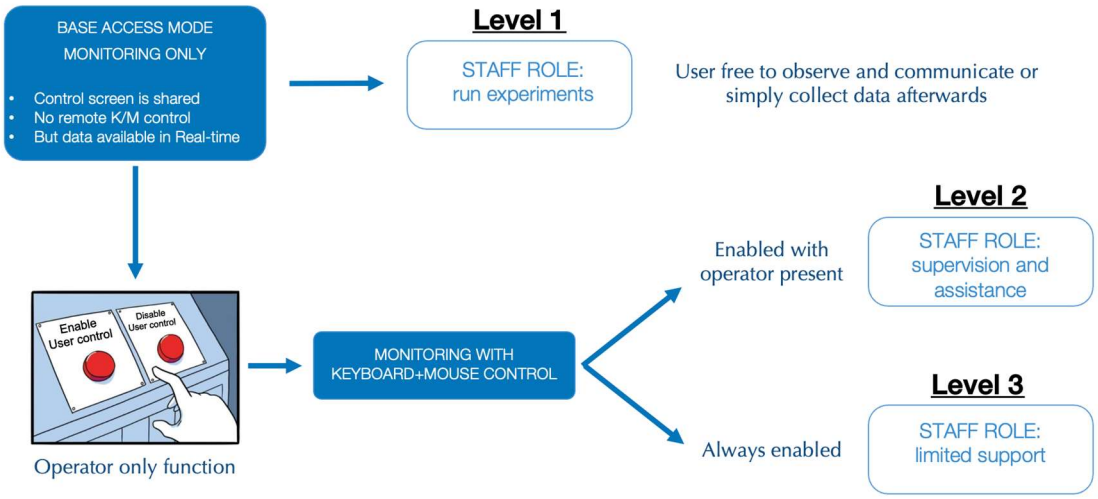

Figure 1: An overview of the three remote access levels.

Appendix: Example user experience questionnaire

R-NMR User Questionnaire

What type of user do you consider yourself?

Beginner/Basic – Advanced – Expert

Do you have any formal training in the acquisition of NMR experimentation?

Any specific classes, vendor courses, in-person training, or relevant practical tuition

What spectrometer brands do you have practical experience with?

Bruker – Varian/Agilent – JEOL – Other (specify)

What types of samples have you worked with?

Sample classes: *Liquids, solids, both*

Sample types: Organic, inorganic, biomolecular

Do you have direct experience of the experiments relevant to your remote access project?
Please provide details:

Do you have experience with modifying pulse sequences?

Please provide details:

Which of the following tasks can you perform independently (y/n)?

Manual insertion of a sample

Automatic insertion of a sample (e.g., using a SampleJet)

Engage the lock (automatically/manually)

Tuner the probe (automatically/manually)

Shim the magnet (automatically/manually)

Calibrate pulses – direct(1H) channel (automatically/manually)

Calibrate pulses – indirect channels (e.g. 13C, 15N, 31P)

Set correct receiver gain (automatically/manually)

Choose a method suitable to your problem (e.g. measuring coupling constants, distance restraints, relaxation rates)

Choose a suitable pulse sequence/parameter set from the standard library of experiments

Optimize the parameters to suit your sample (spectral width, pulse powers and lengths, acquisition time, decoupling power etc.)

Select a suitable method of solvent suppression and optimize the parameters